5-Thia-1-heptanethiol

Inchi: InChI=1S/C6H14S2/c1-2-8-6-4-3-5-7/h7H,2-6H2,1H3
InchiKey: UKCNJCPIHIMVSL-UHFFFAOYSA-N
Formula: C6H14S2
SMILES: CCSCCCCS
Mol. weight [g/mol]: 150.31

Physical Properties

Property code	Value	Unit	Source
gf	62.15	kJ/mol	Joback Method
hf	-86.82	kJ/mol	Joback Method
hfus	19.47	kJ/mol	Joback Method
hvap	42.50	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.450		Crippen Method
mcvol	128.100	ml/mol	McGowan Method
pc	3407.89	kPa	Joback Method
rinpol	1226.00		NIST Webbook
rinpol	1226.00		NIST Webbook
tb	468.32	K	Joback Method
tc	680.70	K	Joback Method
tf	228.24	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.27	J/mol×K	468.32	Joback Method
cpg	264.51	J/mol×K	503.72	Joback Method
cpg	276.18	J/mol×K	539.11	Joback Method
cpg	287.29	J/mol×K	574.51	Joback Method
cpg	297.86	J/mol×K	609.91	Joback Method
cpg	307.88	J/mol×K	645.30	Joback Method
cpg	317.37	J/mol×K	680.70	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R157518&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume